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Accurate atomistic calculations of the Peierls barrier and kink-pair formation energy for <111> screw dislocations in bcc Mo

Multiscale modeling of plastic flow and other mechanical properties in bcc transition metals requires an accurate atomistic description of dislocation energetics as input to larger length scale theories and simulations. Using multi-ion MGPT interatomic potentials derived from first-principles generalized pseudopotential theory, we have recently calculated a wide variety of deformation and defect properties of bcc Mo with considerable success [1], including the equilibrium structure of the <111> screw dislocation core. In the present work, we are using the same MGPT potentials to investigate the energetic barriers to dislocation motion in Mo, including both the full orientation dependence of the Peierls stress required to move an ideal straight <111> screw dislocation and the activation barrier for kink-pair formation in nonstraight screw dislocations. Many-body angular forces, which are accounted for in the present theory through explicit three- and four-ion potentials, are generally important to such properties for the bcc transition metals. This is demonstrated explicitly through calculation of the closely related (110) and (112) gamma surfaces (generalized stacking fault energies). As expected, neither surface displays a stable stacking fault, but the magnitude of the unstable stacking fault energy for the (110) surface is enhanced by 50% over that obtained from a simple radial-force Finnis-Sinclair potential for Mo. By applying various external shear stresses on the relaxed equilibrium <111> screw dislocation core in Mo, we have found the (minimum) ideal Peierls stress for dislocation motion is on the order of 0.02G, where G is the shear modulus of the bulk metal. At the same time, we have found that the calculated Peierls barrier is sensitive to the orientation of the applied stress.

[1] W. Xu and J. A. Moriarty, Phys. Rev. B 54, 6941 (1996).

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